Modern Quantum Mechanics.

Chapter I. Fundamental Concepts

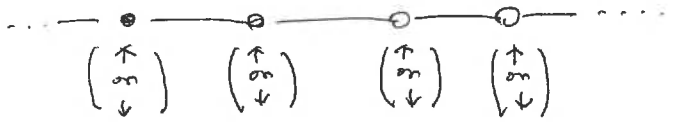
1.1 Hilbert space and State vector

Hilbert space $\xleftarrow{\text{a generalization}}$ Euclidean Space (2D. 3D)

→ can have $\begin{pmatrix} \text{any finite} \\ \text{infinite} \end{pmatrix}$ dim. !

- Hilbert space dimension in QM : examples.

⇒ spin-$\frac{1}{2}$ chain



Q. How many "states" are available ? (accessible)

\# of possible configurations

$= 2^N$ ← dim. of H-space.

⇒ a free particle

"•" (It's just flying in any direction)

↑ "position" : can be anything !

→ H-space dimension : infinite !

cf. what about "momentum" ?

It's conserved.

→ H-space is just a point if $\vec{p}$ is known.
(reduced into)

- What does "a generalization" mean?

- H-space : a vector space.

  ↳ works just like in 2D or 3D Euclidean space.

- In 3D E-space.

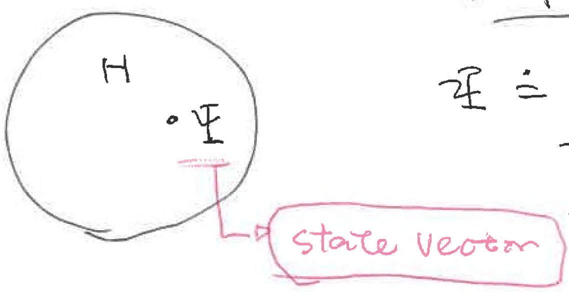
$$\vec{x} \doteq \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \underbrace{x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}_{\text{"basis"}}$$

→ inner products are well-defined!

→ length, angle.

- In H-space.

- ex. spin-½ chain



$$\Psi \doteq a_1 (\uparrow \downarrow \uparrow \cdots) + a_2 (\downarrow \downarrow \uparrow \cdots) + a_3 (\downarrow \uparrow \downarrow \cdots)$$

$\vdots$ many terms.

$a_1, a_2, \cdots$: complex in gen.!

and, the inner products are also defined! ← But, it's a linear combination!

$$(\uparrow \downarrow \uparrow) \perp (\downarrow \downarrow \uparrow)$$

No overlaps! : "orthogonal"

Math.

- formulation of a "state vector"

↳ Bra-Ket notation (Dirac).

1.2 Kets, Bras, Operators.

- H-space : a complex vector space.

(1) a state vector $\doteq$ a "ket" vector $\boxed{|\alpha\rangle}$

works like a "vector".

- addition : $|\gamma\rangle = |\alpha\rangle + |\beta\rangle$
- addition is commutative : $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$

  for all $|\alpha\rangle$ and $|\beta\rangle$.
- there exists a "null" vector $|\emptyset\rangle$.

  $|\alpha\rangle + |\emptyset\rangle = |\emptyset\rangle + |\alpha\rangle = |\alpha\rangle$
- multiplication by any c-number : $|\alpha'\rangle = c|\alpha\rangle$.
- distributive law : $a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a|\beta\rangle$

same concept.

(2) an observable, an operator, an eigenket.

"an observable can be represented by an operator."

$\Rightarrow$ $A|\alpha\rangle$ = another ket, in general.

an operator

"eigen"

- Eigenket $\doteq$ Eigenvector

the same ket

$$A|a_1\rangle = a_1|a_1\rangle, \quad A|a_2\rangle = a_2|a_2\rangle \quad \cdots$$

a number (eigenvalue)

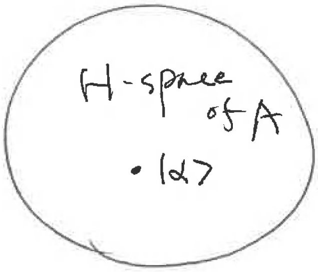
- Eigenstate : a physical state corresponding to an eigenket.

ex. $S_z|S_z;+\rangle = \frac{\hbar}{2}|S_z;+\rangle, \quad S_z|S_z;-\rangle = -\frac{\hbar}{2}|S_z;-\rangle$

⇒ N-dim. H-space of A.

⇐ spanned by N eigenkets of A. $\{|a'\rangle\}$.

∴ " $|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle$ "



(3) Bra space and Inner Products

: is dual to the ket space

$|\alpha\rangle \longleftrightarrow \langle\alpha|$ bra vector

ket vec. Dual Correspondence

If $|\gamma\rangle = c_\alpha|\alpha\rangle + c_\beta|\beta\rangle$,

$\xleftrightarrow{\text{D.C.}} \underbrace{c_\alpha^* \langle\alpha| + c_\beta^* \langle\beta|}_{}$ complex conj.

- Inner product : $\langle\beta|\alpha\rangle = (\langle\beta|)\cdot(|\alpha\rangle)$

⇐ a generalization of $x^T \cdot y$

property 1. $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$: complex conj.

property 2. $\boxed{\langle\alpha|\alpha\rangle} = \langle\alpha|\alpha\rangle^* \boxed{\geq 0.}$

: positive definite metric unless $|\alpha\rangle = |0\rangle$

- This is essential to the probabilistic interpretation of Q.M.

- $|\alpha\rangle$ and $|\beta\rangle$ are orthogonal if $\langle\alpha|\beta\rangle = 0$.

- normalization : $|\tilde{\alpha}\rangle = \dfrac{1}{\left[\sqrt{\langle\alpha|\alpha\rangle}\right]} |\alpha\rangle$

  $\Rightarrow \langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1$.

  ↳ norm of $|\alpha\rangle$

  ~ length of a vector.

(4) Operators.

- equal operators $X = Y$ if $X|\alpha\rangle = Y|\alpha\rangle$ for an arb. ket.

- null operator : $X|\alpha\rangle = 0$.

- cummulative and associative addition

  $X+Y = Y+X$, $X+(Y+Z) = (X+Y)+Z$

- Linear operator : $X(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle$

  (most ops in Q.M.)

- duality :

  $X|\alpha\rangle \xleftrightarrow{\text{D.C.}} \langle\alpha| X^{+}$!

  Hermitian adjoint.

- Hermitian op : $X = X^{+}$

(5) Multiplication. ~ matrix multiplication.

- Noncommutative, in general !

  $XY \neq YX$.

- associative : $X(YZ) = (XY)Z \equiv XYZ$

- $(XY)^{+} = Y^{+}X^{+}$

  because. $X(Y|\alpha\rangle) \xleftrightarrow{\text{D.C.}} (\langle\alpha|Y^{+})X^{+}$ $= (XY)^{+}$

- Outer product of $|\beta\rangle$, $\langle\alpha|$

: $|\beta\rangle\langle\alpha|$ ← This is also an operator.

(c.f. $\langle\alpha|\beta\rangle$ = number)

- illegal products :
  - $X\langle\alpha|$ (×)
  - $|\alpha\rangle X$ (×)
  - $|\alpha\rangle|\beta\rangle$ or $\langle\alpha|\langle\beta|$ (if $|\alpha\rangle, |\beta\rangle$ are in the same H-space)
    (×) (×)

"Nonsense"

(6) Associative Axiom.

- $(|\beta\rangle\langle\alpha|)\cdot|\gamma\rangle = |\beta\rangle\cdot(\langle\alpha|\gamma\rangle)$ ← number

means ↳ it rotates $|\gamma\rangle$ into the direction of $|\beta\rangle$.

- $\langle\beta|X|\alpha\rangle = \langle\beta|\cdot(X|\alpha\rangle) = (\langle\beta|X)\cdot|\alpha\rangle$

- Hermitian ⇒ $\langle\beta|X|\alpha\rangle = \langle\alpha|X|\beta\rangle^*$.

proof.
$$\begin{aligned}\langle\beta|X|\alpha\rangle &= \langle\beta|\cdot(X|\alpha\rangle)\\ &= \left[(\langle\alpha|X^\dagger)\cdot|\beta\rangle\right]^*\\ &= \langle\alpha|X^\dagger|\beta\rangle^* = \langle\alpha|X|\beta\rangle^*\end{aligned}$$
if X is Hermitian

1.3 Base Kets and Matrix representation

(1) Eigenkets of an observable

Theorem Eigenvalues of a Hermitian op : Real

Eigenvectors corrs. diff. eigenvalues
- kets are "orthogonal"!

proof.

Eigenket of A : $\{|a_i\rangle\}$, Eigenvalues : $\{a_i\}$

$\rightarrow$ $A|a_i\rangle = a_i|a_i\rangle$, $\langle a_j|A = a_j^*\langle a_j|$

(A : Hermitian)

Then, $(a_i - a_j^*)\langle a_j|a_i\rangle = 0$.

① if $a_i = a_j$, $a_i = a_j^*$. $\left(\text{since } \langle a_i|a_i\rangle \neq 0\right)$

(eigenvalues are real).

② if $a_i \neq a_j$, $\langle a_j|a_i\rangle = 0$. $\left(\text{since } a_i - a_j^* = a_i - a_j \neq 0\right)$

(orthogonal eigenkets)

Eigenkets are normalized : $\langle a_j|a_i\rangle = \delta_{ij}$. #

(2) Eigenkets as Base kets.

recall : an arbitrary ket $|\alpha\rangle$ in H-space of A .

$\rightarrow$ expansion with the eigenkets of A . ($\{|a\rangle\}$)

$$|\alpha\rangle = \sum_{a'} C_{a'}|a'\rangle .$$

now, we know C_a by $\langle a|\times$

$C_a = \langle a|\alpha\rangle$. $\left(\text{since } \langle a|a'\rangle = \delta_{aa'} \text{ (orthogonality)}\right)$.

Now, one can rewrite $|\alpha\rangle$ as

$$|\alpha\rangle = \sum_a |a\rangle\langle a|\alpha\rangle = \underbrace{\left[\sum_a |a\rangle\langle a|\right]}_{= I \text{ (identity op)}} \cdot |\alpha\rangle$$

$$\sum_a |a\rangle\langle a| = \mathbb{1}$$: completeness relation (closure)

very important.

ex. $\langle\alpha|\alpha\rangle = 1 \rightarrow$ condition for C_a?

$$\langle\alpha|\alpha\rangle = \langle\alpha| \cdot \sum_a |a\rangle\langle a| \cdot |\alpha\rangle$$

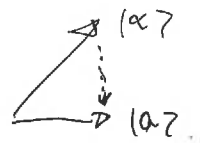
$$= \sum_a |\langle a|\alpha\rangle|^2 = \underline{\sum_a |C_a|^2 = 1}.$$

Another expression with a <u>projection operator</u>.

- <u>projection operator</u> def. $\boxed{\Lambda_a = |a\rangle\langle a|}$

meaning : $\Lambda_a|\alpha\rangle = \langle a|\alpha\rangle\, |a\rangle$

$\rightarrow$ Λ_a selects the portion of the ket $|\alpha\rangle$ parallel to $|a\rangle$.

(
).

Completeness : $\underline{\sum_a \Lambda_a = I}$

(Summing up all proj.s → It has to be "complete".

* for a continuous parameter a,

$$\int da\, |a\rangle\langle a| = \mathbb{1}$$